

Succinic acid, 2-isopropoxyphenyl 2-methylbutyl ester

Inchi:	InChI=1S/C18H26O5/c1-5-14(4)12-21-17(19)10-11-18(20)23-16-9-7-6-8-15(16)22-13(2)3
InchiKey:	ICIFLVRFLTZQNN-UHFFFAOYSA-N
Formula:	C18H26O5
SMILES:	CCC(C)COC(=O)CCC(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]:	322.40

Physical Properties

Property code	Value	Unit	Source
gf	-374.26	kJ/mol	Joback Method
hf	-822.17	kJ/mol	Joback Method
hfus	35.74	kJ/mol	Joback Method
hvap	78.55	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.749		Crippen Method
mvol	261.470	ml/mol	McGowan Method
pc	1551.22	kPa	Joback Method
rinpol	2224.00		NIST Webbook
rinpol	2224.00		NIST Webbook
tb	817.02	K	Joback Method
tc	1021.36	K	Joback Method
tf	468.11	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.08	J/molxK	817.02	Joback Method
cpg	806.64	J/molxK	851.08	Joback Method
cpg	821.03	J/molxK	885.13	Joback Method
cpg	834.26	J/molxK	919.19	Joback Method
cpg	846.33	J/molxK	953.25	Joback Method
cpg	857.24	J/molxK	987.30	Joback Method
cpg	867.00	J/molxK	1021.36	Joback Method
dvisc	0.0006591	Paxs	468.11	Joback Method

dvisc	0.0003307	Paxs	526.26	Joback Method
dvisc	0.0001903	Paxs	584.41	Joback Method
dvisc	0.0001211	Paxs	642.57	Joback Method
dvisc	0.0000830	Paxs	700.72	Joback Method
dvisc	0.0000603	Paxs	758.87	Joback Method
dvisc	0.0000459	Paxs	817.02	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357968&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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